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Valence Offsets of Three Series of Alloy Heterojunctions *

ZHENG Jin-cheng(郑金成), WANG Ren-zhi(王仁智),
ZHENG Yong-mei(郑永梅), CAI Shu-hui(蔡淑惠)
Department of Physics, Xiamen University, Xiamen 361005

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Electron structure of three series of alloy heterojunctions $(GaAs)_x(Ge_2)_{1-x}/Ge$, $(AlAs)_x(Ge_2)_{1-x}/Ge$ and $Al_xG_{1-x}As/Ge$ are calculated by linear muffin-tin orbital method with atomic-sphere approximation using the average-bond-energy theory in conjunction with a cluster expansion method. The results indicate the variations of $\Delta E_v(x)$ at heterojunctions $(GeAs)_x(Ge_2)_{1-x}/Ge$ and $(AlAs)_x(Ge_2)_{1-x}/Ge$ are nonlinear, which are very different from that of $Al_xGa_{1-x}As/Ge$.

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The valence-band offsets (VBO, i. e., ΔE_v) at semiconductor heterointerfaces are the most important parameters in determining the electrical and optical properties of heterojunctions and superlattices. Because of its importance, this topic has stimulated a great deal of experimental and theoretical research work recently. There is much experimental and theoretical work for ΔE_v at heterojunctions constructed by element or compound semiconductors presented in recent years, but theoretical studies on $\Delta E_v(x)$ at alloy-type heterojunctions (ATHJs) are still very scarce. We have presented a theoretical method of calculating $\Delta E_v(x)$ of lattice-match alloy heterojunctions such as $Al_xGa_{1-x}As/GaAs$,[2] $In_xGa_{1-x}As/In_xAl_{1-x}As$ (Ref. 3) and lattice-dismatch such as $In_xGa_{1-x}As/GaAs$,[4] which is made up of the average bond energy method in conjunction with the cluster expansion method, based on the linear muffin-tin orbital method with atomic-sphere approximation (LMTO-ASA) band-structure method.

It is shown that the average bond energy method in conjunction with the cluster expansion method is well fit to the calculation of $\Delta E_v(x)$ at alloy-type heterojunctions.

In this paper, using the theoretical method we calculate the VBO of three typical lattice-matched ternary alloy heterojunctions $(GaAs)_x(Ge_2)_{1-x}/Ge$, $(AlAs)_x(Ge_2)_{1-x}/Ge$ and $Al_xGa_{1-x}As/Ge$ and compare the theoretical results with the relevant experimental data.

In this paper, the band structures of ternary alloy $(GaAs)_l(Ge_2)_{4-l}$, $(AlAs)_l(Ge_2)_{4-l}$ and $Al_lGa_{4-l}As_4$ are calculated with LMTO-ASA method. Among the five ordered structures ($l = 0, 1, 2, 3, 4$), which correspond to the composition $x = 0, 0.25, 0.5, 0.75, 1.0$ in ATHJ, respectively, $l = 0$ and 4 are zinc-blende (ZB) structure, $l = 2$ is CuAu structure (labeled by $L1_0$) and $l = 1$ and 3 are Luzonite ($L1_2$) structures.[5] The lattice constants of five ordered structures can be obtained as the average of the bulk materials GaAs, AlAs and Ge in proportion to contents according to Vegard's law.[6] The special-K-point method[7] is adopted for the summation over the Brillouin zone. Two special K points are used for ZB and $L1_0$ structures and only one special K point is used for the $L1_2$ structure.[2,3] After getting the self-consistent band structures for the five ordered structures, the average bond energy[2] can be obtained as following:

$$E_m^l = \frac{1}{2MN}\sum_{n=1}^{2M}\sum_k E_n^l(k)\,, \tag{1}$$

where N is the number of unit cells and M the number of valence bands, l is the label of five ordered structures. For the ZB, $L1_0$, and $L1_2$ structures, M is evaluated by 4, 8, and 16,

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respectively. From the results of band calculation (i.e., valence-band maximum E_{v}^{l}) and average bond energy E_{m}^{l} of the five ordered structures, one can obtained valence-band maximum and average bond energy of ATHJ by the cluster expansion[2] are:

$$E_{\mathrm{m}}(x) = \sum_{l} P_l(x) E_{\mathrm{m}}^{l}\,, \tag{2}$$

$$E_{\mathrm{v}}(x) = \sum_{l} P_l(x) E_{\mathrm{v}}^{l}\,, \tag{3}$$

where the statistic weight $P_l(x) = \binom{4}{l} x^l (1-x)^{4-l}$ is the possibility of the l short region ordered structure taking place in the alloy. The plot of the statistic weight $P_l(x)$ is showed in Fig. 1.

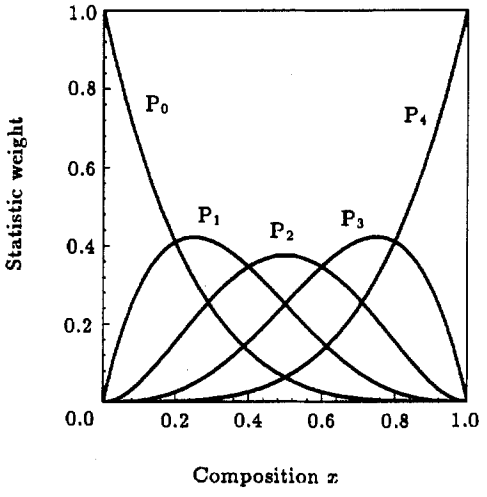

Fig. 1. Plot of the statistic weight $P_l(x)$.

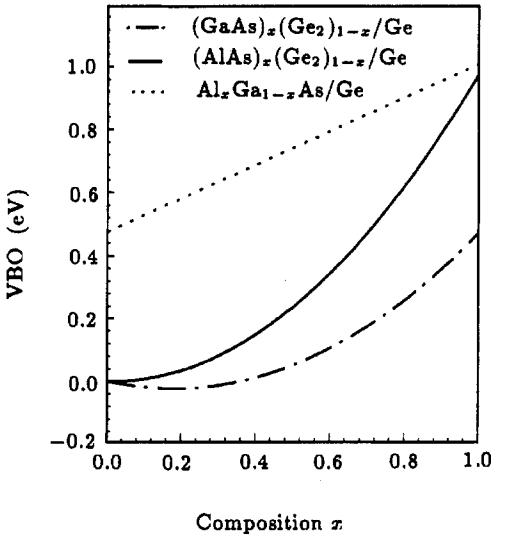

Fig. 2. VBO at the ATHJ heterojunctions $(\mathrm{GaAs})_x(\mathrm{Ge_2})_{1-x}/\mathrm{Ge}$, $(\mathrm{AlAs})_x(\mathrm{Ge_2})_{1-x}/\mathrm{Ge}$, and $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As/Ge}$ as function of the alloy composition x.

The $\Delta E_{\mathrm{v}}(x)$ value can be obtained by aligning the average bond energy in materials A and B,[2]

$$\Delta E_{\mathrm{v}}(x) = [E_{\mathrm{v}}^{B}(x) - E_{\mathrm{m}}^{B}(x)] - [E_{\mathrm{v}}^{A}(x) - E_{\mathrm{m}}^{A}(x)]\,. \tag{4}$$

The values $\Delta E_{\mathrm{v}}(x)$ at the three-component alloy $(\mathrm{GaAs})_x(\mathrm{Ge_2})_{1-x}/\mathrm{Ge}$, $(\mathrm{AlAs})_x(\mathrm{Ge_2})_{1-x}/\mathrm{Ge}$, and $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As/Ge}$ heterojunctions can be determinated by using Eq. (7), which are shown as the regressed two-order polynomials:

$$(\mathrm{GaAs})_x(\mathrm{Ge_2})_{1-x}/\mathrm{Ge} : \Delta E_{\mathrm{v}}(x) = 0.737x^2 - 0.269x\,, \tag{5}$$

$$(\mathrm{AlAs})_x(\mathrm{Ge_2})_{1-x}/\mathrm{Ge} : \Delta E_{\mathrm{v}}(x) = 1.032x^2 - 0.031x\,, \tag{6}$$

$$\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As/Ge} : \Delta E_{\mathrm{v}}(x) = -0.002x^2 + 0.532x + 0.475\,. \tag{7}$$

In the above expressions, we can see that the $\Delta E_{\mathrm{v}}(x)$ values of these heterojunctions are functions of x, Fig. 2 shows the $\Delta E_{\mathrm{v}}(x)$ curves of $(\mathrm{GaAs})_x(\mathrm{Ge_2})_{1-x}/\mathrm{Ge}$, $(\mathrm{AlAs})_x(\mathrm{Ge_2})_{1-x}/\mathrm{Ge}$,

and $Al_xGa_{1-x}As/Ge$ as functions of composition x.

From Fig. 2, one can see that the VBO of three series of alloy heterojunctions is a function of composition x, and the VBOs of $(AlAs)_x(Ge_2)_{1-x}/Ge$ and $Al_xGa_{1-x}As/Ge$ increase with x increasing, namely, with the increasing of the AlAs content (i. e., with the decreasing of Ge content). But the VBO of $(GaAs)_x(Ge_2)_{1-x}/Ge$ decreases with x increasing at $0 < x < 0.182$, then increases with x increasing at $0.182 < x < 1.0$. At the same value of composition, the VBO of $(AlAs)_x(Ge_2)_{1-x}/Ge$ is larger than that of $(GaAs)_x(Ge_2)_{1-x}/Ge$, and that of $Al_xGa_{1-x}As/Ge$ is the largest. The dependence of the VBO at $(AlAs)_x(Ge_2)_{1-x}/Ge$ and $(GaAs)_x(Ge_2)_{1-x}/Ge$ on the composition x is in large nonlinearity, but the variation of VBO at $Al_xGa_{1-x}As/Ge$ with the composition x is almost linear. Equations 5–7 show that the two-order coefficient which is a characterization of bending of $\Delta E_v(x)$ curve of three series of alloy heterojunctions is different. The two-order coefficients of $(GaAs)_x(Ge_2)_{1-x}/Ge$ and $(AlAs)_x(Ge_2)_{1-x}/Ge$ are 0.737 and 1.032 respectively, but that of $Al_xGa_{1-x}As/Ge$ is very small, it is only 0.002. It implies that the $\Delta E_v(x)$ values of the alloy heterojunctions $Al_xGa_{1-x}As/Ge$ can be obtained approximately by linear regressing from the ΔE_v values of the bulk material heterojunctions GaAs/Ge and AlAs/Ge, but the VBOs of $(GaAs)_x(Ge_2)_{1-x}/Ge$ and $(AlAs)_x(Ge_2)_{1-x}/Ge$ cannot be got by linear regressing. This behavior makes the $(GaAs)_x(Ge_2)_{1-x}/Ge$ and $(AlAs)_x(Ge_2)_{1-x}/Ge$ systems as $(\text{III V})_x(\text{VI}_2)_{1-x}/(\text{III V})$ type, but very different from the system $Al_xGa_{1-x}As/Ge$ as $(\text{III V})_x(\text{III V})_{1-x}/(\text{III V})$ type. Therefore, one can change the composition of alloy heterojunctions to tailor and design the electronic band structure conveniently.

Comparing our results with the experiment data, we find that our results are in good agreement with the experiment data. Present result for GaAs/Ge is 0.475, the experiment result 0.56, model solid 0.59,[8] selfconsistent supercell calculation (SCSC) 0.46,[9] selfconsistent dipole model (SCD) 0.45,[10] Harrision's tight-binding "pinned" model (HAO) 0.66,[11] charge-neutrality- point model (CNP) 0.32,[12] dielectric-midgap-energy model (DME) 0.45.[13] Our result for AlAs/Ge is 1.0, the experiment result 0.95, model solid 1.19,[8] SCSC 1.03,[9] SCD 1.08,[10] HAO 0.78,[11] CNP 0.87,[12] DME 0.84.[13] The theoretical prediction remains to be tested by further experimental data.

In conclusion, we studied the electronic structure of three series of alloy heterojunctions $(GaAs)_x(Ge_2)_{1-x}/Ge$, $(AlAs)_x(Ge_2)_{1-x}/Ge$ and $Al_xGa_{1-x}As/Ge$ by LMTO-ASA method using the average-bond-energy theory in conjunction with a cluster expansion method. The results indicate the variations of $\Delta E_v(x)$ at heterojunctions $(GaAs)_x(Ge_2)_{1-x}/Ge$ and $(AlAs)_x(Ge_2)_{1-x}/Ge$ are nonlinear, which are very different from that of $Al_xGa_{1-x}As/Ge$, the partly theoretical result is in good agreement with the experimental data and other theoretical results.

REFERENCES

[1] R.Z. Wang and M. C. Huang, Sci. China, A 36 (1993) 319.
[2] R. Z. Wang, S. H. Ke and M. C. Huang, Phys. Rev. B 51 (1995) 1935.
[3] J. C. Zheng, Y. M. Zheng and R. Z. Wang, Chin. Sci. Bulletin, 41 (1996) 2050.
[4] S. H. Ke, R. Z. Wang and M. C. Huang, Solid State Commun. 95 (1995) 95.
[5] W. R. L. Lambrecht and B. Segall, Phys. Rev. B 47 (1993) 9289.
[6] L. Vegard, Z. Phys. 5 (1921) 17.
[7] D. J. Chadi and M. L. Cohen, Phys. Rev. B 8 (1973) 5747.
[8] C. G. Van de Walle and R. M. Martin, Phys. Rev. B 35 (1987) 8154.
[9] E. N. Christensen, Phys. Rev. B 37 (1988) 4528.
[10] W. R. L. Lambrecht and B. Segall, Phys. Rev. B 41 (1990) 2813.
[11] W. A. Harrison and J. Tersoff, J. Vac. Sci. Technol. B 4 (1986) 1068.
[12] J. Tersoff, J. Vac. Sci. Technol. B 4 (1986) 1066.
[13] M. Cardona and N. E. Christensen, Phys. Rev. B 35 (1987) 6182.